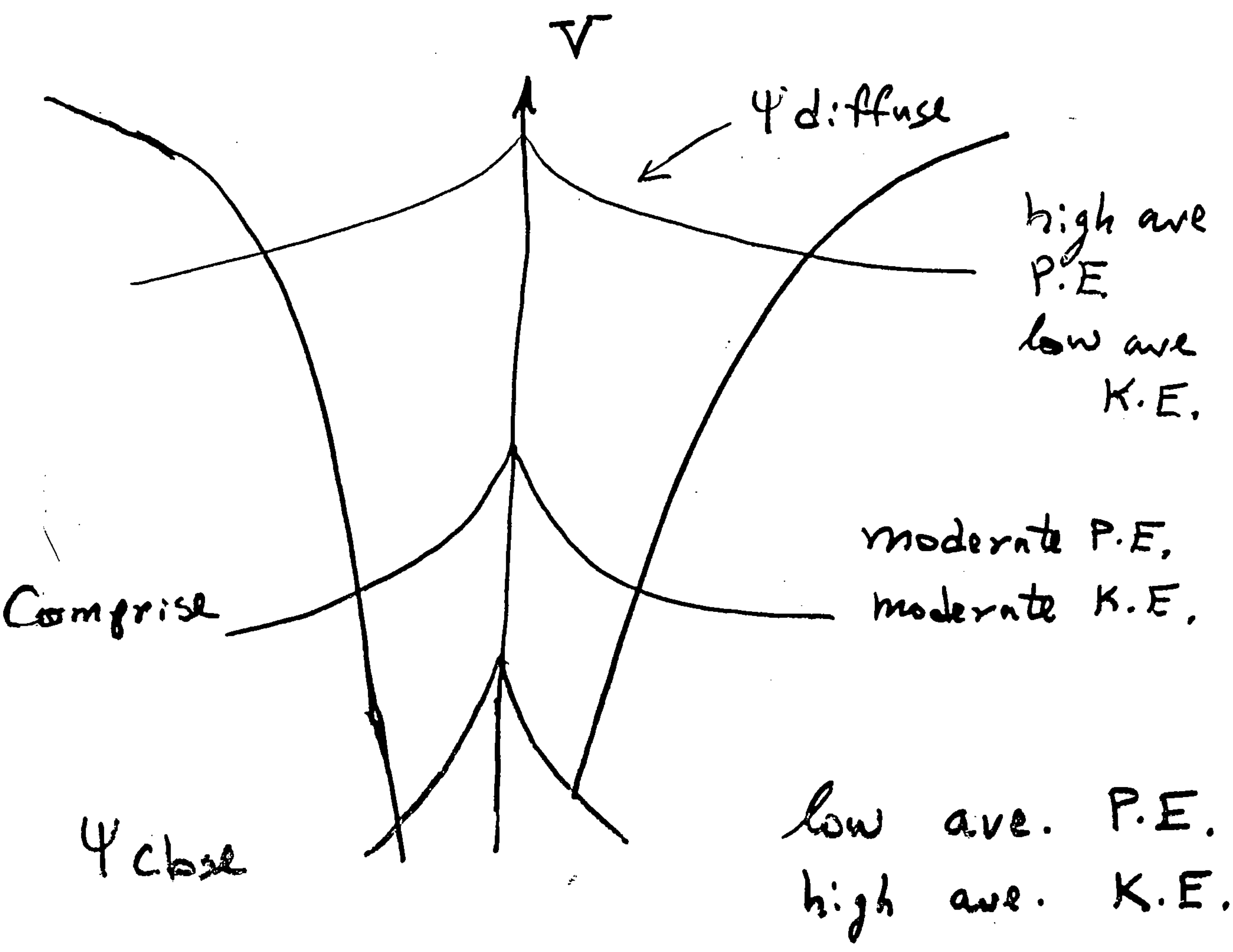
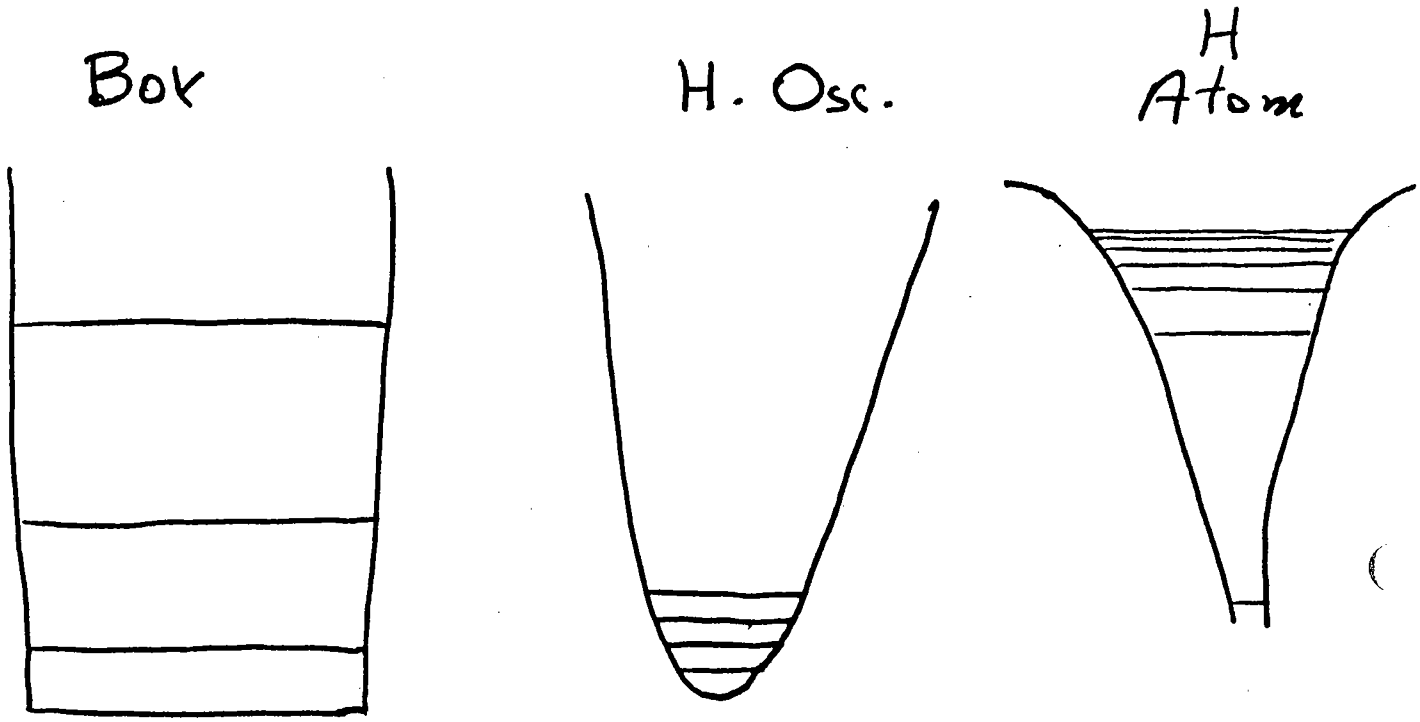
Consider $l = 0$ — the K.E. arises due to movement in r (through the nucleus)



ground state when $n=1$ $(l=0)$

as n increases : the electron becomes less tightly bound and therefore the energy is higher

Consider The Dependence of Energy on the Quantum Numbers



$E \propto n^2$ $\qquad\qquad$ v $\qquad\qquad$ $-\frac{1}{n^2}$

Hydrogen Atom (cont)

$$\Psi(r,\theta,\varphi) = R_{n,l}(r)\,\underbrace{\Theta_{l,m_l}(\theta)\,\Phi_{m_l}(\varphi)}_{Y_{l,m_l}}$$

The Quantum numbers have dependent ranges of values:

$$n = 1, 2, 3, \ldots$$

$$l = 0, 1, 2, \ldots (n-1) \quad \text{——} \quad s, p, d, \ldots$$

$$m_l = -l, -l+1, \ldots 0, 1, \ldots l$$

back to last page

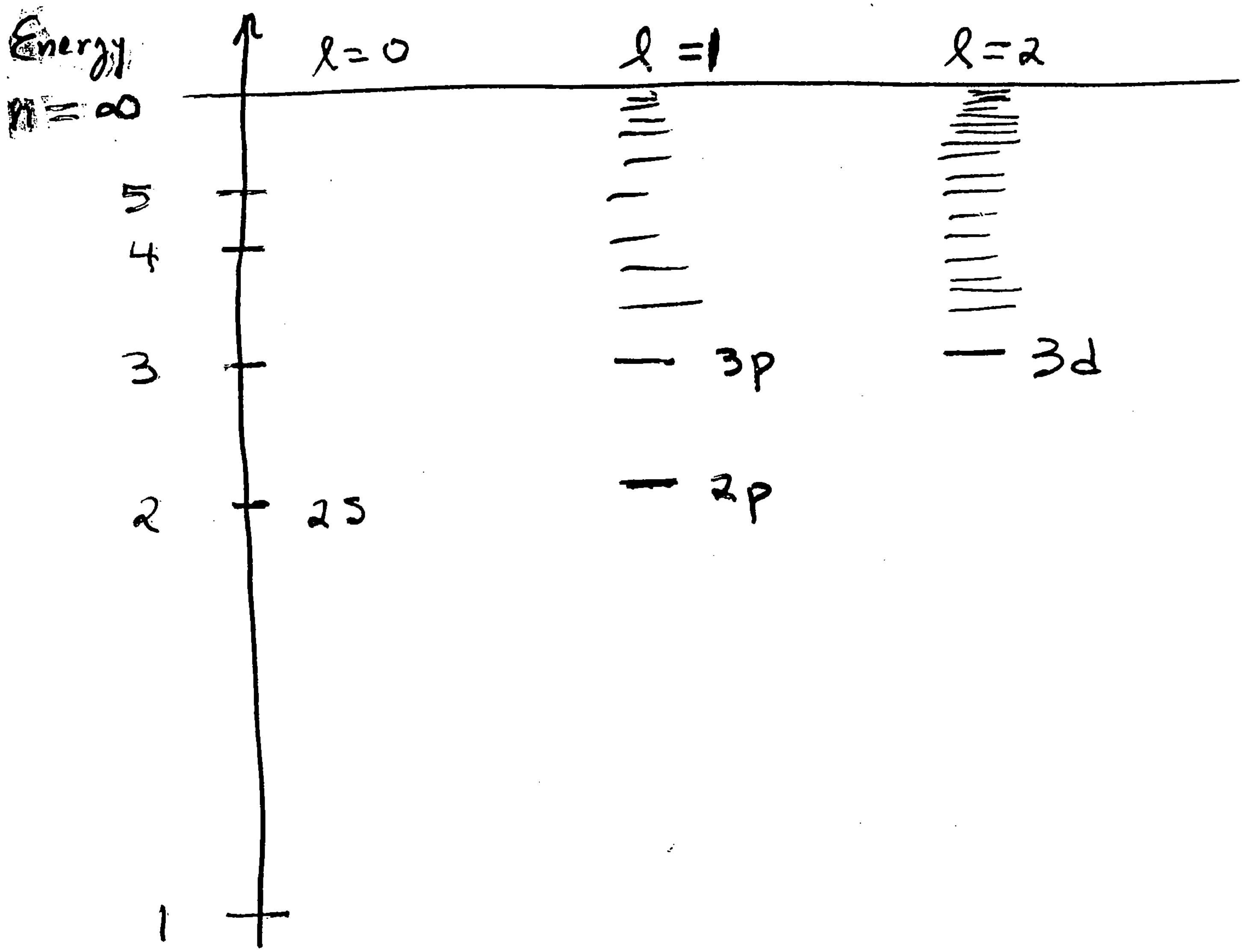
Consider The Ranges of Quantum Numbers

n	l	m_l	g_n	name
1	0	0	1	1s
2	0	0	4	2s
2	1	0		$2p_0$
2	1	−1		$2p_{-1}$
2	1	+1		$2p_{+1}$
3	0	0	9	3s
3	1	0		$3p_0$
3	1	−1		$3p_{-1}$
3	1	+1		$3p_{+1}$
3	2	0		$3d_0$
3	2	−1		$3d_{-1}$
3	2	+1		$3d_{+1}$
3	2	−2		$3d_{-2}$
3	2	+2		$3d_{+2}$

$\Psi_{2p_0}, \Psi_{2p_{+1}}, \Psi_{2p_{-1}}$ Involves exponential solutions in m_l

$\Psi_{2p_x}, \Psi_{2p_y}, \Psi_{2p_z}$ Sin, Cos solutions

H atom (Continued)



Consider $Y_{\ell, m_\ell}(\theta, \varphi)$

Motion of a particle on a sphere.

$Y_{0,0}$ = Constant

$\therefore$ no dependence on θ, φ

no angular momentum

$\therefore$ n s — are spherically symmetric

$$\psi_{1s} = \underbrace{\frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2}}_{\text{normalizing constant}} \underbrace{e^{-Zr/a_0}}_{\text{decaying exponential}}$$

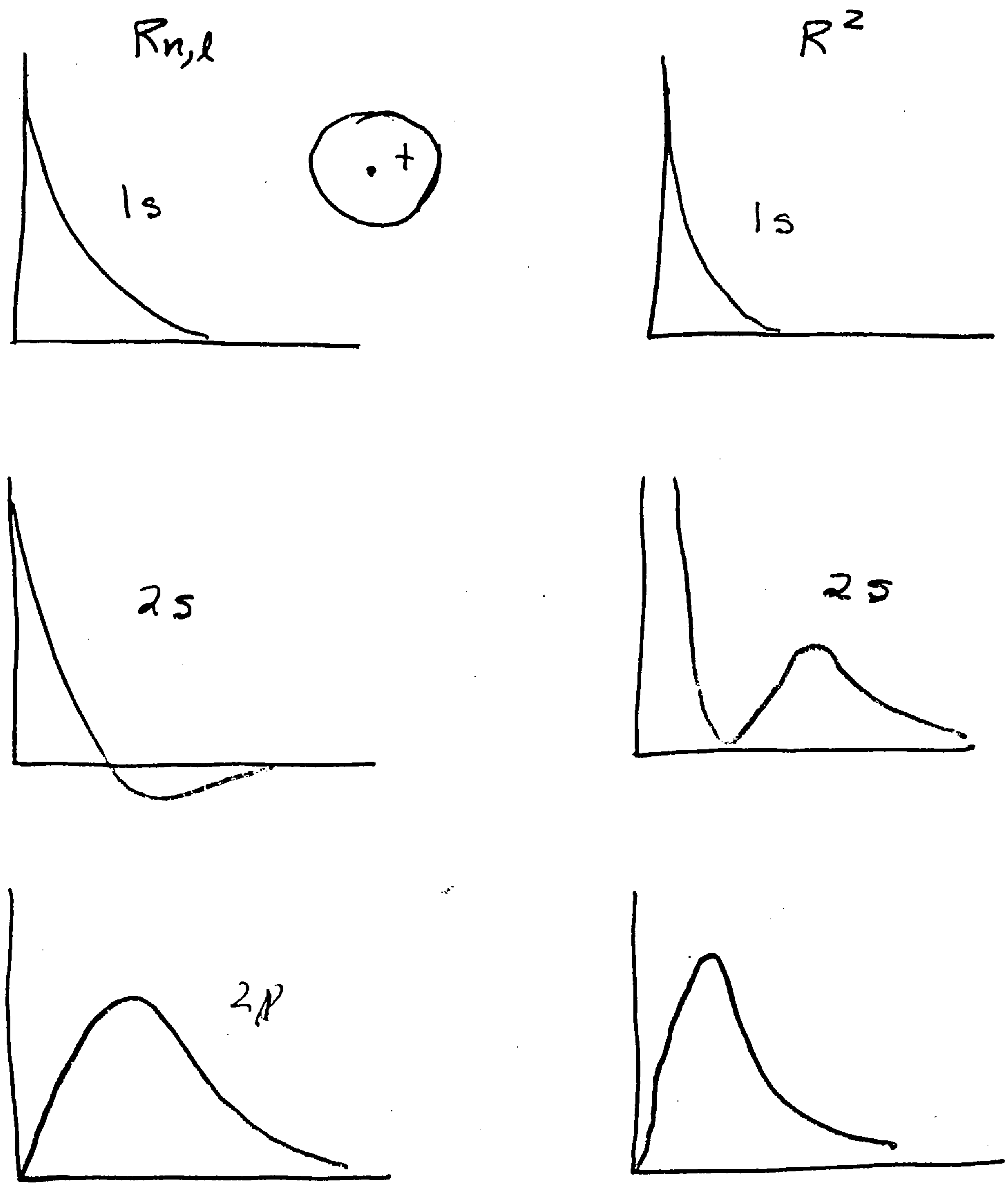
always +

$\Rightarrow 1$ at $r = 0$

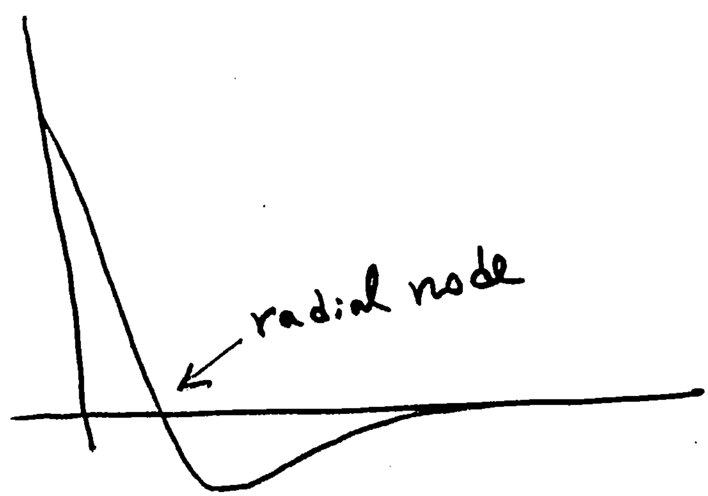
$\Rightarrow 0$ as $r \Rightarrow \infty$

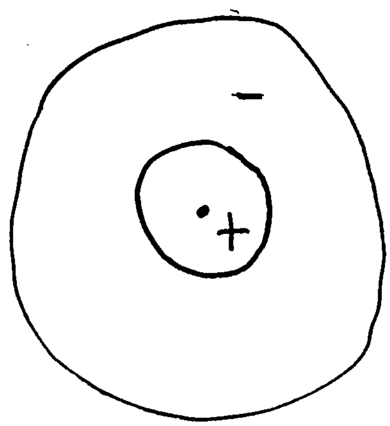
Hydrogen Atom

$$\psi_{n,l,m_l}(r) = R_{n,l}\, Y_{l,m_l}$$



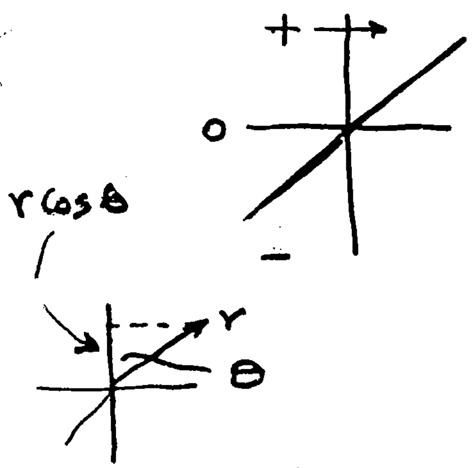
$$\Psi_{2s} = \underbrace{\frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{5/2}}_{\text{Norm. Constant}} \underbrace{\left(2 - \frac{Zr}{a_0}\right)}_{\substack{\text{small } r \Rightarrow + \\ \text{large } r \Rightarrow -}} \underbrace{e^{-Zr/2a_0}}_{\text{always} \geq 0}$$



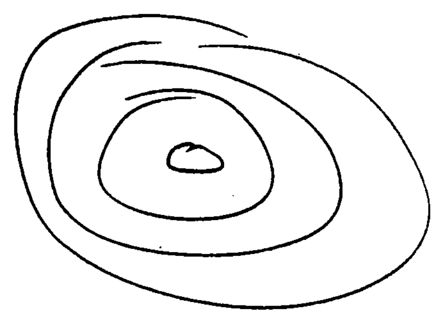


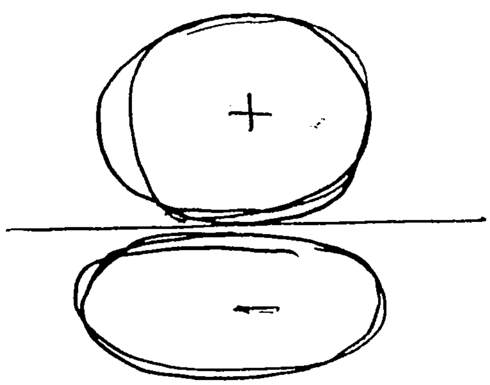
$$\psi_{2p_0} = \underbrace{\frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{5/2}}_{\text{Norm. Const.}} \underbrace{r\cos\theta}_{z} \underbrace{e^{-Zr/2a_0}}_{\text{Spherical}}$$

$\therefore$ $2p_0$ AO result of multiplying spherical functions (decaying exponentially) by $f(z)$



times





0 where $z = 0$

$2p_z$ – directional properties $\Rightarrow z$

$$\Psi_{2p_{+1}} = f(\theta, \varphi, r) \Rightarrow$$ involves exponentials in φ

$$\Psi_{p_{-1}} = f'(\theta, \varphi, r) \Rightarrow$$

Combine $\Psi_{p_{+1}}$ and $\Psi_{p_{-1}}$

by sum and difference

<u>obtain</u>

Ψ_{2p_x}

Ψ_{2p_y}

P-orbitals obtained
for $\ell = 1$

d - orbitals obtained $\ell = 2$

$$m_\ell = +2, +1, 0, -1, -2$$

$\therefore$ degeneracy $= 2\ell+1 = 5$

$\exp(0) \Rightarrow$ real

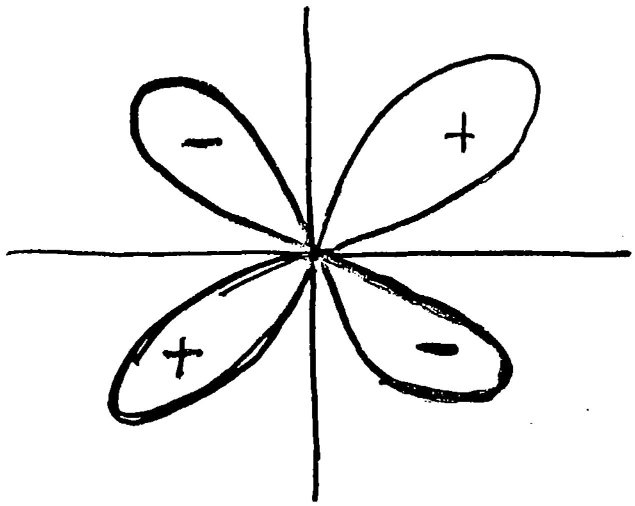
All others are complex

$\therefore$ add / sub. to obtain real functions

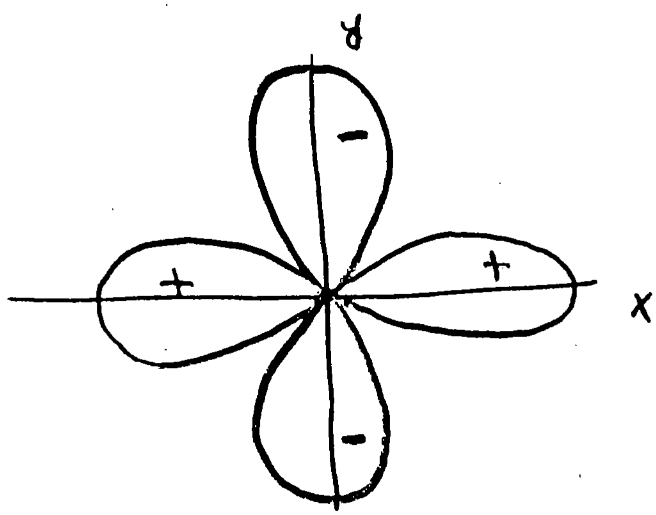
$\pm 1 \Rightarrow \cos\phi, \sin\phi$

$\pm 2 \Rightarrow \cos 2\phi, \sin 2\phi$

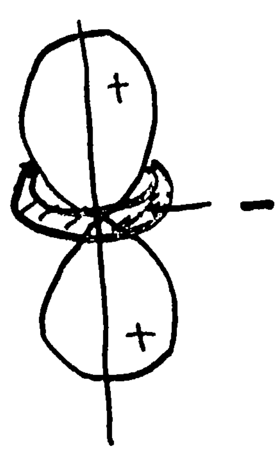
d – orbitals



$3d_{xz}$, $3d_{yz}$



$3d_{x^2-y^2}$



$3d_{z^2}$